Giant Enhancements in Electronic Transport and Photoelectric Properties of Bismuth Oxysulfide by Pressure-driven 2D-3D Structural Reconstruction

Wenge Yang[1]* and Ganghua Zhang[1,2]

[1]*Center for High Pressure Science and Technology Advanced Research (HPSTAR), Shanghai, P.R. China*
[2]*Shanghai Research Institute of Mterials, Shanghai 200437, P.R. China*
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*e-mail: yangwg@hpstar.ac.cn

Layered bismuth oxychalcogenides have been considered as exciting material systems with potential applications in superconductor and thermoelectricity, but their optoelectronic properties still require greater diligence. The pressure-driven 2D–3D structural reconstruction is an efficient strategy to in-situ turn the electronic configuration of functional materials, and yet has remained a challenge for both fundamental studies and technological applications. With aids of synchrotron X-ray diffraction, in-situ high pressure optical observation of light transmission, electric conductivity, and photocurrent measurements, we uncovered the dramatic enhancements in the electronic transport and phototelectric properties with the pressure tuning effect on this layered materials. Unlike the pressure induced structure phase transition in many other materials, we noticed the pressure-driven buckling effect of the layered bismuth oxysulfide $Bi_9O_{7.5}S_6$ to a 3D network structure. Although no crystallographic symmetry change was observed up to 58.1 GPa, the layer and bonding distances between and within BiO and BiS layer change dramatically, which drives the enhancements of electric conductivity by 6 orders of magnitude, increasing of photocurrent by 4 orders of magnitude, and significant narrowing down of band gap from 1.34 to 0.45 eV. These findings may open a new avenue for discovering and designing high-efficiency photodetectors and energy-harvesting materials.

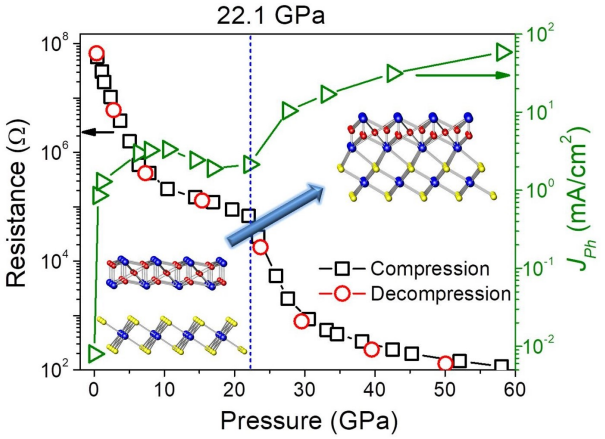

Figure 1. Structural evolutions and enhancements on the conductivity and photocurrent at pressures up to 58.1 GPa. Below 21 GPa, the overall crystalline structure is still layered while the distance between BiO and BiS layer schrinkes with pressure increasing, with first stage enhancement of conductivity and photocurrent; above 21 GPa, a 2D to 3D buckling takes place and second stage enhancements show more pronounced behavior.

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[1] G. Zhang, Q. Zhang, Q. Hu, B. Wang andd W. Yang J. *Mater. Chem. A,* 2019, **7,** 4019.
[2] G. Zhang, F. Liu, T. Gu, Y. Zhao, N. Li, W. Yang, and S. Feng, *Adv. Electon. Mater.* 2017, **3,** 1600498.